There is no simulation of n-qubit operations by a single Hamiltonian with 2-spin interaction

Torsten Asselmeyer-Maluga, Matthias Kolbe, and Helge Rosé
FhG FIRST, Kekuléstr. 7, 12489 Berlin, Germany
(Dated: February 1, 2008)

Today's devices for quantum computing are still far from implementing useful and powerful quantum algorithms. Decoherence and the wish to resist the effects of errors in a system of quantum bits incurs a lot of overhead in the number of gates and qubits. From a theoretical perspective, controlled quantum simulation raises the hope to simulate the unitary quantum operationes generated by a Hamiltonian with 3-body interaction with a suitably designed element that is constructed of only 2-body interactions. That replacement would happen without any additional gates, and its possibility would be due to the ambiguity of the unit element of the Lie group connected with the algebra of traceless hermitian matrices. We show that this hope is void, and give a general proof for this for any order of interaction.

arXiv:quant-ph/0508029v1 3 Aug 2005

INTRODUCTION

The outstanding properties of exponentiality, fast access, universality, branching and interference in connection with complex amplitudes as a whole give reason to hope that new classes of problems can be solved with quantum computation in contrast to the conventional von-Neumann machines [1, 2]. However, in all those optimistic visisons of straight-forward developments of quantum computing, one has to face the unavoidable effects of decoherence. Nowadays, in the presence of the broadly investigated field of error correction, the view in dealing with the difficulties of decoherence could be too optimistic. In particular, a high amount of entanglement, which seems to be essential for good quantum algorithms, is very sensitive for decoherence effects [3]. Of course, it is indeed possible to protect quantum states against unwanted influences with error correcting codes and fault-tolerant quantum algorithms, but there is a high price to be paid in an enormous overhead of gates and qubits required to store and proceed redundant information. This overhead is acceptable however as long as the error rate per gate, the accuracy threshhold, is under a certain critical value [4, 5].

A rough estimation of the gate number required for implementing the quantum fourier transformation (see [6] for instance), which is a major component in Shor's well known factoring algorithm [7], shows that for n qubits no fewer than n Hardarmard gates plus $\frac{1}{2}(n^2 - n)$ controlled phase gates are required [6]. For the more essential Modulo operation, many more gates, at the order of n^3 [8], have to be considered. So for a useful factorization of a big number, say of 1000 bits, it is very likely that hundreds of millions of gates need to be applied, and this number will be further increased massively (albeit polynominally) by error correction. Very recent investigation shows how architecture [8] and error correction [9] affect the computation time of Shor's algorithm. Ion-trap experiments, being good realization candidates, show gate operation times from $10^{-14}\,$s up to microseconds, whereas typical decoherence time τ is about one second. Recent experiments by the group of Rainer Blatt in Innsbruck [10] come up with $\tau = 10\,$s for ^{40}Ca-Ions. In nuclear magnetic resonance (NMR) experiments, another very good candidate, decoherence time could be even much longer, up to 10^8 seconds, but the operation time per gate also increases to milliseconds [6]. Lloyd mentions decoherence time for NMR in such a long range as years [11] under optimal conditions. Of course, these values show that up to 10^{14} operations and more might be possible in these systems, but only under really optimal circumstances. However, the mutually influences of decoherence, error correction, gate count, qubit count, accuracy threshhold and operation time (all in strong architectural dependency) results in a situtation that seems to be far from implementing really practical and powerful quantum algorithms within large quantum systems and realistic decoherence times.

But not only these rather technical restriction have to be taken into account for realizing a quantum computer. As we shall outline, the operations that act on multiple qubits simultaniously, which occur in various algorithms, are generated from unphysical Hamiltonians as well. The standard construction method of taking logarithms of unitary operators reveals Hamiltonians with multipartite interaction terms. Of course, arbitrary n-bit quantum gates can be expressed as compositions of 2-bit quantum gates, and this universality is well developed in its basics [12, 13, 14, 15, 16, 17, 18] and optimizations (see for instance the work of Zhang et al. [19, 20, 21, 22]). Unfortunately, this happens at the cost of increasing gate numbers, which is critical as outlined above. Wouldn't it be nice to have a replacement of such Hamiltonians by a single realistic one? There appears to be hope to do so, as we will discuss in the next section, but in the rest of the paper we shall prove the contrary.

CONSTRUCTING HAMILTONIANS FROM UNITARY OPERATIONS

In the following we will introduce the problem of the representation of a unitary operation (as an element of the unitary group $U(2^n)$) by the exponential of a suitable Hamiltonian (as an element of the Lie algebra $\mathfrak{u}(2^n)$). As an example we consider the CNOT operation represented by the unitary matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

also given by the Lie algebra element

$$it\,H = i\frac{\pi}{4}(\mathbb{1} - \sigma_z) \otimes (\mathbb{1} - \sigma_x)$$

where σ_x, σ_z are the Pauli matrices and $\mathbb{1}$ is the 2×2 unit matrix. From the physical point of view, every unitary operation must be generated by a Hamiltonian with respect to a special time. In our example we have

$$CNOT = \exp(iHt)$$

with $t = \pi/4$ and $H_{CNOT} = (\mathbb{1}-\sigma_z)\otimes(\mathbb{1}-\sigma_x) = \sigma_z\otimes\sigma_x - \sigma_z\otimes\mathbb{1} - \mathbb{1}\otimes\sigma_x + \mathbb{1}\otimes\mathbb{1}$. This Hamiltonian can be physically interpreted as a spin system with 2-spin interaction given by $\sigma_z\otimes\sigma_x$ in an exterior field $\sigma_z\otimes\mathbb{1}+\mathbb{1}\otimes\sigma_x$. For a 3-qubit operation like the Toffoli gate we obtain ($t = \pi/8$):

$$\begin{aligned} H_T &= (\mathbb{1} - \sigma_z) \otimes (\mathbb{1} - \sigma_z) \otimes (\mathbb{1} - \sigma_x) \\ &= \mathbb{1} \otimes (\mathbb{1} - \sigma_z) \otimes (\mathbb{1} - \sigma_x) \\ &\quad - (\sigma_z \otimes \mathbb{1} \otimes \mathbb{1}) + (\sigma_z \otimes \mathbb{1} \otimes \sigma_x) \\ &\quad + (\sigma_z \otimes \sigma_z \otimes \mathbb{1}) - (\sigma_z \otimes \sigma_z \otimes \sigma_x) \end{aligned}$$

and thus a 3-spin interaction $\sigma_z \otimes \sigma_z \otimes \sigma_x$. But an interaction between 3 constituents is artificial in nature [31] and only possible under very restricted conditions.

Representations of Hamiltonians in terms of eigenenergies may be related to representations in terms of Pauli spin matrices σ_z much more generally [23]. Assume an Hamiltonian in its eigenstructure. It can be written as

$$H = \sum_{k=0}^{\infty} \varepsilon_k |\psi_k\rangle\langle\psi_k|.$$

Here, the $|\psi_k\rangle$ are the complete set of orthogonal eigenstates and the $\{\varepsilon_i\}$ are the energy eigenvalues. For simulation in an n-qubit system let us truncate the sum to the first 2^n ernergie levels. Then we have

$$\begin{aligned} H &= \sum_{k=0}^{2^n-1} \varepsilon_k |\psi_k\rangle\langle\psi_k| \\ &= \sum_{k=0}^{2^n-1} \alpha_k \, (\sigma_z)^{\nu_1^k} \otimes (\sigma_z)^{\nu_2^k} \otimes \cdots \otimes (\sigma_z)^{\nu_n^k}, \end{aligned}$$

where the $\{\alpha_i\}$ are real numbers representing coupling strength and the $\{\nu_i^k\}$ are the binary representation digits for the integer k, thus take on the values $\{0, 1\}$. It turns out that the vectors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\alpha}$ are related by the matrix equation $\boldsymbol{\varepsilon} = \boldsymbol{M}\boldsymbol{\alpha}$ with $\boldsymbol{M}$ as the Hardamard matrix for n qubits. For example, for two qubits, we have:

$$\boldsymbol{M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

Once the arbitrary Hamiltonian is expressed in terms of many-body interactions $\sigma_z \otimes \sigma_z \otimes \cdots \otimes \sigma_z$, it can be broken down in terms of available external and internal (two-body) Hamiltonians. Control theory enables us, furthermore, to simulate arbitrary Hamiltonians by those that are predetermined by some appropriate experiment [24].

At this point we want to briefly introduce the decomposition techniques of Khaneja et al. [25, 26] as an interesting theoretical approach to universality. Assume an element of the special unitary group describing qubit evolution, $U \in SU(2^n)$. It is always possible to decompose it into $U = K_1 A K_2$ where $K_1, K_2 \in SU(2^{n-1}) \otimes SU(2^{n-1}) \otimes U(1)$ as long as A is an element of the so-called Cartan subalgebra of the Riemann symmetric space

$$\frac{SU(2^n)}{SU(2^{n-1}) \otimes SU(2^{n-1}) \otimes U(1)}.$$

One should note that this is recursive, because then we can further decompose K_1 and K_2 in $SU(2^{n-2}) \otimes SU(2^{n-2}) \otimes U(1)$ and so on, down to elements of $SU(2) \otimes SU(2)$. This decomposition ist based on the parametrization of $SU(2^n)$ with canonical parameters of the second kind [27]. Suppose $U \in SU(2)$, then we can express any element in two ways

1. $U = \exp\left[-i(\alpha_1\sigma_x + \alpha_2\sigma_y + \alpha_3\sigma_z)\right]$
2. $U = \exp(-i\beta_1\sigma_x)\exp(-i\beta_2\sigma_y)\exp(-i\beta_3\sigma_z)$

with $\alpha_i, \beta_i \in \mathbb{R}$. This coincides with the two kinds of canonical parameters, and it would be promising to look for an decomposition technique that suits the first of the above standart parameterizations. Actually, such a decomposition is the goal of our investigation to implement a 3-qubit operation with a single 2-particle Hamiltonian. Remember that in the case of $SU(8)$, terms of 3-particle interations (like in the Toffoli-Hamiltonian above) and terms of 2-particle interactions are orthogonal in their algebra $\mathfrak{su}(8)$ as they are different basis elements. Based on that fact our goal may appear out of reach, but there is an ambiguity in the exponential!

Consider the eigenvalues $\lambda_1, \ldots, \lambda_{2^n}$ of the Hamiltonian H and the unitary matrix A of eigenvectors diagonalizing $H = A(diag(\lambda_1, \ldots, \lambda_{2^n}))A^+$. Then the exponential $\exp(iHt)$ can be written as

$$\exp(iHt) = A(diag(e^{i\lambda_1 t}, \ldots, e^{i\lambda_{2^n} t}))A^+$$

and we can shift every eigenvalue $\lambda_k t + 2\pi n_k$ by an integer n_k so that the exponential is unchanged. We denote this shift by

$$N = 2\pi A(diag(n_1, \ldots, n_{2^n}))A^+$$

with $[H, N] = 0$ and $\exp(iN) = \mathbb{1}$. Thus, we obtain

$$\exp(iHt) = \exp(iHt + iN)\,.$$

Now we consider a 3-qubit system. Let H be a Hamiltonian with 3-spin interactions and h a Hamiltonian with 2-spin interactions defined for a 3-qubit system. By the ambiguity above, there is perhaps a shift N so that

$$\begin{aligned} Ht = ht' + N &\Longrightarrow \exp(iHt - iht') = \exp(iN) = \mathbb{1} \\ &\Longrightarrow \exp(iHt) = \exp(iht') = U \end{aligned}$$

and we ask for the existence of such a shift N with $[(Ht - ht'),\ N] = 0$. We want to emphasize here that this is not a trivial question and it is not obvious what's coming out at the end. Anyhow, we must dispel the hope that such an N exists and we will prove it for any order in the next section.

THE NO-GO THEOREM

In this section we will consider the following situation: an n-qubit system with state space $\mathbb{C}^{2^n}$ and a unitary operation U lying in $U(2^n)$. Furthermore, we have a Hamiltonian H with n-spin interaction and a Hamiltonian h with $(n{-}1)$-spin interaction. Assume

$$U = \exp(iH)\,,$$

then we will show that there is no Hamiltonian h with

$$U = \exp(iH) = \exp(ih)\,,$$

i.e. every unitary operation $U \in U(2^n)$ can only be represented by a Hamiltonian with n-spin interaction. For a warm-up example, we start with the first non-trivial case $n = 2$ and state that no unitary 2-qubit operation U generated by H can be also generated by h. To prove this we begin with the assumption that by definition the exponential of a 2-spin interaction given by $H = \sigma_i \otimes \sigma_j$, $i, j \in \{x, y, z\}$, can never be decomposed as

$$\exp(\sigma_i \otimes \sigma_j) \neq A \otimes B \qquad A, B \in U(2)\,, \tag{1}$$

otherwise the 2-qubit operation is decomposible by 1-qubit operations. Furthermore, every 1-spin "interaction" is given by $h = \sigma_j \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_i$, and we have

$$\begin{aligned} \exp(ih) &= \exp\left[i(\sigma_j \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_i)\right] \\ &= \exp(i\sigma_j \otimes \mathbb{1})\exp(i\mathbb{1} \otimes \sigma_i) \\ &= \exp(i\sigma_j) \otimes \mathbb{1})(\mathbb{1} \otimes \exp(i\sigma_i) \\ &= \exp(i\sigma_j) \otimes \exp(i\sigma_i)\,, \end{aligned}$$

but that contradicts (1).

We showed that no non-trivial unitary operation generated by 2-spin interactions can also be generated by 1-spin interactions (which physically represents an exterior field that acts on the spin system). Ok, this might be no suprise because no interaction whatsoever was allowed here.

No-Go-Theorem for Hamiltonian representations: *No unitary n-qubit operation U $(n > 2)$ generated by a Hamiltonian H with n-spin interactions can be generated by a Hamiltonian h with $(n{-}1)$-spin interactions as well so that the relation*

$$U = \exp(iH) = \exp(ih) \tag{2}$$

is fulfilled.

PROOF: Consider a Hamiltonian H_{2^n} as an element of the Lie algebra $\mathfrak{u}(2^n)$ and a Hamiltonian H_{2^n-1} as an element of the Lie algebra $\mathfrak{u}(2^n - 1)$. We will prove that an element U of the unitary group $U(2^n)$ generated by H_{2^n} can never be generated by $E(H_{2^n-1})$ with respect to all embeddings $E : \mathfrak{u}(2^n - 1) \to \mathfrak{u}(2^n)$. Then the theorem follows by using 2^{n-1} times that result. In the following we use the abbreviation $k = 2^n$.

Consider a family of Hamiltonians $H_k(a_1, \ldots, a_{k^2})$ parametrized by k^2 parameters which is the dimension of the Lie algebra $\mathfrak{u}(k)$, i.e. we have a map $H_k : U(k) \to \mathfrak{u}(k)$ from the coordinates of the Lie group (seen as smooth manifold with group operation) to the Lie algebra (seen as tangent space of the Lie group) [27]. The tangent bundle $TU(k)$ of the Lie group is trivial, i.e. $TU(k) = U(k) \times \mathfrak{u}(k)$. Thus the map H_k extends to a map $H_k : U(k) \to TU(k)$, i.e. H_k is a vector field on $U(k)$. By the same argument we can interpret H_{k-1} as a vector field on $U(k-1)$. By the simple algebraic argument of linear independence, both vector fields H_k and $E(H_{k-1})$ disagree, i.e.

$$H_k \neq E(H_{k-1})\,. \tag{3}$$

By using the assumption (2) and the linear independence (3) we have

$$\exp(iH_k) = \exp\left[iE(H_{k-1})\right] \Longrightarrow H_k - E(H_{k-1}) = N_k\,,$$

where N_k is a vector field that depends on $k^2 - (k-1)^2 = 2k - 1$ parameters. Then we can interpret the vector field N_k as vector field on $U(k)$ modulo $U(k-1)$ or as vector field on the coset space $U(k)/U(k{-}1)$, i.e. for a fixed H_k, the variation of N_k with respect to $E(H_{k-1})$ is expressed by this coset space $U(k)/U(k-1)$. The definition of this space is given by the fact that the group $U(k-1)$ acts on $U(k)$, and two elements $g_1, g_2 \in U(k)$ are said to be equivalent if and only if an element $G \in U(k-1)$ with $g_2 = Gg_1$ exists. Then the equivalence classes are denoted by $U(k)/U(k-1)$. It is a well-known fact [28] that $U(k)/U(k{-}1) = S^{2k-1}$, i.e. the $(2k{-}1)$-dimensional

sphere. Now, if we can show that the vector field N_k vanish at some point then we can shift this vanishing point at every place to show that

$$H_k - E(H_{k-1}) = 0\,,$$

thus contradicting the linear independence of H_k and $E(H_{k-1})$ (see (3) above). Thus we are looking for the existence of a non-vanishing vector field on $U(k)/U(k-1) = S^{2k-1}$ that represents N_k. By a famous mathematical result of Adams [29], there is only a non-vanishing vector field on S^{2k-1} for $k = 1, 2, 4$. The vector fields on all other spheres vanish in one point, which would contradict (3). The cases $k = 1, 2$ are trivial, and $k = 4$ is covered by our warm-up example. That completes the proof. **qed**

CONCLUSION

Based on the fact that there is an ambiguity of the unit element of a Lie group connected with its Lie algebra, the hope is raised that elements of $SU(2^n)$ generated by Hamiltonians of $\mathfrak{su}(2^n)$ carrying n-body interactions can also be generated by Hamiltonians carrying at most $(n-1)$-body interactions. The ambiguity can be interpreted as equivalence classes represented by multidimensional spheres. Therefore, by transferring this problem to a geometrical view and treating Hamiltonians as vector fields on the group, we could show that the hope of replacing unphysical multi-particle interactions is void. The central idea of the proof is the theorem of Adams [29] about vanishing vector fields on spheres. The degree of interaction, which is produced by the logarithm of a unitary operation, cannot be reduced. Thus, for n-qubit operations, n-body interactions are needed. The only way to avoid those interactions is the decomposition of unitary operations in terms of universal 2-qubit gates for the price of a higher number of operations. With this insight we want to challenge the theory of adiabatic quantum computing [30], which heavily relies on the implementation of 3-body interactions. Therefore, we want to notice that the realization of the ideas of adiabatic computing is daring if not impossible.

This work was supported by the BMBF under the project number 01IBB01A. We thank Dominik Janzing, Andreas Schramm and Martin Wilkens for useful hints and discussions.

[1] D. Deutsch and R.Josza, Proceedings of the Royal Society London A **439**, 553 (1992).
[2] E. Bernstein and U. Vazirani, SIAM J. Comput. **26**, 1411 (1997), URL `citeseer.ist.psu.edu/bernstein97quantum.html`.
[3] J. Preskill, Proceedings of the Royal Society London A **454**, 469 (1998).
[4] E. Knill, R. Laflamme, and W. Zurek, pre-print: quant-ph/9610011 (1996).
[5] J. Preskill, pre-print: quant-ph/9712048 (1997).
[6] M. A. Nielsen and I. L. Chuang, *Quantum Computing And Quantum Information* (Cambrige University Press, 2000).
[7] P. W. Shor, SIAM Journal on Computing **26**, 1484 (1997), URL `citeseer.ist.psu.edu/185210.html`.
[8] R. V. Meter, K. M. Itoh, and T. D. Ladd, preprint: quant-ph/0507023 (2005).
[9] S. J. Devitt, A. G. Fowler, and L. C. Hollenberg, preprint: quant-ph/0408081 (2004).
[10] A. Kreuter et al., pre-print: physics/0409038 (2004).
[11] S. Lloyd, preprint: quant-ph/9912086 (1999).
[12] A. Barenco, D. Deutsch, A. Ekert, and R. Jozsa, Physical Review Letters **74**, 4083 (1995).
[13] D. Deutsch, A. Barenco, and A. Ekert, Proceedings of the Royal Society London A **449**, 669 (1995).
[14] D. P. DiVincenzo and J. Smolin, Physical Review A **51**, 1015 (1995).
[15] T. Sleator and H. Weinfurter, Physical Review Letters **74**, 4087 (1995).
[16] A. Barenco, Proceedings of the Royal Society London A **449**, 678 (1995).
[17] D. P. DiVincenzo, Physical Review A **51**, 1015 (1995).
[18] S. Lloyd, Physical Review Letters **75**, 346 (1995).
[19] J. Zhang, J. Vala, K. B. Whaley, and S. Sastry, Physical Review A **67** (2003).
[20] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, Physical Review Letters **91** (2003).
[21] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, Physical Review A **93** (2004).
[22] Y. Zhang, L. H. Kauffman, and M.-L. Ge, pre-print: quant-ph/0502015 (2005).
[23] C. H. Tseng, S. Somaroo, Y. Sharf, E. Knill, R. Laflamme, T. F. Havel, and D. G. Cory, Physical Review A **61**, 012302 (1999).
[24] P. Wocjan, M. Roetteler, D. Janzing, and T. Beth, Quantum Information and Computation **2**, 133 (2002).
[25] N. Khaneja and S. Glaser, pre-print: quant-ph/0010100 (2000).
[26] N. Khaneja, R. Brockett, and S. Glaser, Physical Review A **63**, 032308 (2001).
[27] A. Sagle and R. Walde, *Introduction to Lie groups and Lie algebras* (Academic Press, New York and London, 1973).
[28] M. Nakahara, *Geometry and Topology for physicists* (Adam Hilger, Bristol and New York, 1989).
[29] J. Adams, Ann. of Math. **75**, 603 (1962).
[30] D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, pre-print: quant-ph/0405098 (2004).
[31] It follows from first principles that matter is represented by fermions given mathematically as Dirac spinors and fulfilling the Dirac equation. Interaction between two fermions is only given by introducing a gauge field which coupled to the Dirac spinor. But that kind of coupling leads to a 2-particle interaction.